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DR. WALTER E. MYERS

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AFOSR - IX - 89-17

**First International Conference on the Structure of Surfaces (ICSOS-1)**  
**Berkeley, California**  
**August 13-16, 1984**  
**Schedule of Presentations**

All *oral sessions* will be held in the Sibley Auditorium of the Bechtel Engineering Center of the University of California campus.

All *poster sessions* and *coffee breaks* will be held in Room 120, one floor below Sibley Auditorium.

INV indicates invited presentations.

**Monday, August 13, 1984 (Deadline for Manuscript Submission)**

- 8:00-17:30 Registration in lobby by Sibley Auditorium (Also 8:00-17:30 August 14-16)
- 8:30-18:00 First half of commercial exhibit—Room 120
- 8:30 A3 INV S.Y. Tong  
INTRODUCTION—S.Y. Tong
- 8:40 A1 INV F. Jona  
Determination of Surface Structure by LEED
- 8:40 A2 INV M. Aono, R. Souda, C. Oshima and Y. Ishizawa  
Structure Analysis of Semiconductor and Inorganic Compound Surfaces  
by Impact Collision Ion Scattering Spectroscopy
- 9:20 A3 INV J. Tersoff  
Theory of the Scanning Tunneling Microscope
- 10:00 COFFEE BREAK—Room 120
- 10:50-12:10 B. CLEAN METALS—J.R. Smith, Presiding
- 10:50 B1 INV M. Rocca, H. Ibach, S. Lehwald, B.M. Hall, M.L. Xu and S.Y. Tong  
Electron-Phonon Scattering and Structure Analysis
- 11:10 B2 INV J.C. Lapujoulaude, B. Salanon and D. Gorse  
Surface Structure Analysis by Atomic Beam Diffraction
- 11:50 B3 INV J.R. Noonan and H.L. Davis  
Several Faces of Aluminum
- 12:10-14:00 LUNCH BREAK
- 14:00-16:00 C. MOLECULAR ADSORPTION I—A.M. Bradshaw, Presiding
- 14:00 C1 INV T.H. Upton  
Determining Molecular Adsorbate Structures from Adsorbate Electronic Properties
- 14:40 C2 INV M.A. Van Hove  
Structure Determination of Molecular Adsorbates with Dynamical LEED and HREELS
- 15:20 C3 INV J. Stöhr  
SEXAFS and NEXAFS Studies of Chemisorbed Molecules: Bonding and Structure
- 16:00-18:00 D. TECHNIQUES, ORDERING—posters (and refreshments)—Room 120
- D1 P.H. Fuoss and A. Fischer-Colbrie  
Structural Studies of Ultra-Thin Amorphous Layers on Surfaces
- D2 K.S. Liang, P.H. Fuoss, G.J. Hughes and P. Eisenberger  
Synchrotron X-Ray Scattering Study of Chemisorption System: Oxygen on Cu(110) Surface
- D3 K.H. Lee, M.H. Lee and H.I. Zhang  
Boundary and Size Effects on Frequencies of a Finite Simple Cubic  
Lattice with Coherently Adsorbed Surface Layers

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AFOSR  
1984-12-12

- D4 R.H. Howell, P. Meyer, I.J. Rosenberg and M.J. Fluss  
A New Capability for the Study of Surfaces with Intense Positron Beams
- D5 H.G. LeDuc, A.P. Thakoor, J. Lambe and S.K. Khanna  
Influence of Adsorbates on Surface States of (111) Gold Observed by Electron Tunneling and Electroreflectance
- D6 A.N. Jette, C.B. Bargeron and B.H. Nall  
Dynamical Computations of Current Image Diffraction Images (CID)
- D7 T. Hsu and J.M. Cowley  
REM Studies of Crystal Lattice Terminations at Surfaces
- D8 S. Ferrer and C. Ocal  
Electronic Properties of Small Gold Deposits on Very Thin Aluminum Oxide Layers. The Appearance of Subsurface Gold
- D9 C.R. Aita, C.J. Kubiak, N.C. Tran and T.L. Barr  
X-Ray Photoelectron Loss Spectroscopy of Wide Energy Band Gap Aluminum Compounds
- D10 I. Bartoš and J. Koukal  
On the Role of Space Inhomogeneity of Electron Damping in LEED
- D11 R. Mayol, F. Salvat and J. Parellada-Sabata  
Attenuation of Isotropically Emitted Electron Beams
- D12 K. Müller and K. Heinz  
Computer Controlled LEED Intensity and Spot Profile Determination
- D13 N.C. Bartelt, T.L. Einstein and L.D. Roelofs  
Structure Factors for Adsorbed Overlays from Monte Carlo and Convenient Methods for Analysis of LEED Data Near Phase Transitions
- D14 J.M. Pimbley, P. Fenter and T.-M. Lu  
Short Range Correlations in Imperfect Surfaces and Overlays
- D15 D. Saloner and M.G. Lagally  
Domain-Size Determination in Heteroepitaxial Systems from LEED Angular Profiles
- D16 D.D. Vvedensky, D.K. Saldin and J.B. Pendry  
Near-Edge X-Ray Absorption Spectroscopy
- D17 D.K. Saldin, D.D. Vvedensky and J.B. Pendry  
The Structure of Organic Adsorbates from Elastic Diffuse LEED
- D18 M. Drechsler  
The Structure of Faces and Steps on Hexagonal Metals
- D19 E.A. Conrad, D.S. Kaufman, R. Aten and T. Engel  
Quantitative Studies of Stepped Ni and Cu Surfaces Using Helium Diffraction
- D20 P.R. Pukite, C.S. Lent and P.I. Cohen  
Diffraction From A Disordered Staircase
- D21 F.F. Abraham  
Computer Simulations of Surfaces, Interfaces and Physisorbed Films
- D22 J.C. Campuzano, M.S. Foster, R.F. Willis and W. Unertl  
Determination of the Critical Exponents of the Au(110)(1×2)↔(1×1) Phase Transition
- D23 S.C. Ying and G.Y. Hu  
Theory of Commensurate-Incommensurate Phase Transitions on H/W(001)
- D24 R.J. Behm, K. Christmann, G. Ertl, V. Penka and R. Schwankner  
Competing Reconstruction Mechanisms in H/Ni(110)
- D25 T. Aruga, H. Tochihara and Y. Murata  
Low-Energy Electron Diffraction Studies of K Monolayers on Cu(001)
- D26 K.M. Martini, S. Burdick, M. El-Batanouny and G. Kirczenow  
Molecular Dynamics Investigation of Dislocation-Depinning Transitions in Mismatched Overlays
- D27 S.M. Levine and S.H. Garofalini  
Molecular Dynamics Simulations of Pt Adatoms on the Vitreous Silica Surface



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Tuesday, August 14, 1984

- 8:30-18:00 Continuation of first half of exhibit.
- 8:30-10:10 *E. DISORDER, DEFECTS*—M.B. Webb, Presiding
- 8:30 E1 INV *J.B. Pendry and D.K. Saldin*  
LEED, XANES and the Structure of Disordered Surfaces
- 9:10 E2 *M. Ringger, H.R. Hidber, R. Schlögl, P. Oelhafen, H.-J. Güntherodt, K. Wandelt and G. Ertl*  
The Surface Topography of a Pd Single Crystal Studied by the Scanning Tunneling Microscope
- 9:30 E3 INV *M. Henzler*  
Quantitative Analysis of Spot Profiles of LEED
- 10:10-10:40 COFFEE BREAK—Room 120
- 10:40-12:00 *F. STRUCTURAL TECHNIQUES II*—W.E. Spicer, Presiding
- 10:40 F1 INV *C.J. Wright*  
Surface Characterization by the Inelastic Scattering of Neutrons from Adsorbates
- 11:20 F2 INV *C.P. Slichter*  
NMR and Surface Structure
- 11:40 F3 *W.F. Egelhoff, Jr.*  
X-Ray Photoelectron and Auger Electron Forward Scattering: A New Tool for Studying Epitaxial Growth and Core-Level Binding-Energy Shifts
- 12:00-14:00 LUNCH BREAK
- 14:00-16:00 *G. MOLECULAR ADSORPTION II*—G.A. Somorjai, Presiding
- 14:00 G1 INV *T.E. Maday*  
The Uses and Limitations of ESDIAD for Determining the Structure of Surface Molecules
- 14:40 G2 *A. Puschmann, K.C. Prince, J. Haase, G. Paolucci and A.M. Bradshaw*  
Photoemission and SEXAFS Studies of Oxygen Overlayers on Ag(110)
- 15:00 G3 INV *N.V. Richardson*  
The Characterization of Adsorbed Molecules by Electron Energy Loss Spectroscopy
- 15:40 G4 INV *Y.R. Shen*  
Optical Second-Harmonic Generation for Surface Studies
- 16:00-18:00 *H. SEMICONDUCTORS, INSULATORS*—posters (and refreshments)—Room 120
- H1 *I.P. Batra, F.J. Himpsel, P. Marcus, R. Tromp, M.R. Cook, F. Jona, and H. Liu*  
Structure of Si(111) Surfaces
- H2 *R.M. Tromp, L. Smit and J.F. van der Veen*  
Ion Beam Analysis of the Si(111)-(2×1) Surface
- H3 *R.M. Tromp and E.J. van Loenen*  
Evaluation of Si(111)-(7×7) Structure Models by Channeling and Blocking
- H4 *C.D. Chen, A. Selloni and E. Tosatti*  
Structure and Temperature Dependent Polaron Shifts on Si(111) 2×1
- H5 *Y.S. Shu, W.S. Yang, F. Jona and P.M. Marcus*  
Refinement of the Buckled Dimer Model for Si(001)2×1
- H6 *B.W. Holland, C.B. Duke and A. Paton*  
The Atomic Geometry of Si(100)-(2×1): Resolution of Incompatibility between ELEED and Ion Scattering
- H7 *D.C. Allan and E.J. Mele*  
Surface Vibrational Excitations for Si(100)2×1
- H8 *A. Sakai, M.J. Cardillo, W.R. Lambert, P. Trevor and J. Tersoff*  
The Structures of the Ge(100) and Si(100) Surfaces as Probed by He Diffraction

- H9 H.H. Farrell, J.Q. Broughton, F. Stucki and J.C. Bean  
 Shape Resonances in OH/Semiconductor Systems
- H10 A. Taleb-Ibrahimi, C. Sébenne and F. Proix  
 Metal Induced Reconstructions on Cleaved Silicon (111) at Room Temperature
- H11 G. Le Lay and J.P. Bibérian  
 Metal-Induced Reconstructions of Silicon, Germanium and Diamond Low-Index Surfaces
- H12 S.B. Zhang, J.E. Northrup and M.L. Cohen  
 Theory of the Structure of the Ge-Si(111) Interface
- H13 J.A. Yarmoff and R.S. Williams  
 Low-Energy Ion-Backscattering Angular Distributions from Clean and Absorbate-Covered Ge Surfaces
- H14 M.A. Olmstead and N.M. Amer  
 Polarization Dependent Ge and Si(111) Surface State Optical Absorption: A Probe of Surface Structure
- H15 J.E. Northrup  
 The Arsenic Terminated Ge(111) Surface
- H16 Y.N. Xu, K.M. Zhang and X.D. Xie  
 Studies on the Fermi Level Pinning of GaAs(110) Surfaces
- H17 F. Bartels and W. Mönnich  
 Chemisorption of Oxygen at Cleaved GaAs(110) Surfaces: Work Function and Surface Band-Bending
- H18 O. Nishikawa, O. Kaneda, M. Shibata and E. Nomura  
 Atom-Probe Study of Al-Ga Exchange Reaction on GaAs Surfaces
- H19 G. Xu, W.N. Mei and S.Y. Tong  
 A Vacancy-Buckling Model for the (2×2) GaAs(111) Surface
- H20 R.D. Bringans and R.Z. Bachrach  
 A Comparison between the Electronic Properties of GaAs(111) and GaAs(111)
- H21 P. Hren, D.W. Tu and A. Kahn  
 Atomic Structure of GaAs(211)
- H22 C.B. Duke, C. Mailhiot, A. Paton, K. Li, C. Bonapace and A. Kahn  
 Atomic Geometries of (1×1) Sb Overlays on GaAs(110) and InP(110)
- H23 R.L. Johnson, J.H. Fock, J. Bohr, R. Feidenhansl, J. Als-Nielsen, M. Nielsen and M. Toney  
 Surface X-Ray Diffraction from the Polar (111) Surfaces of InSb
- H24 L. Smit, T.E. Derry and J.F. van der Veen  
 Atomic Structure of Clean and Al Covered III-V Compound Cleavage Faces
- H25 J.M. Nicol, J. Howard and J. Eckert  
 IR and Neutron Spectroscopy of Hydrogen and Ethylene Adsorbed on Type A Zeolites
- H26 J. Eckert, B.H. Grier, L. Passell, H. Patterson, D. Richter and R. Rollefson  
 Structures and Dynamics of Ethylene Surface Layers on Graphite
- H27 N.J. Wu and A. Ignatiev  
 C(0001)-(2\*2)K Surface Intercalated Structure

18:30 Dinner meeting for International Organizing Committee. Faculty Club, Berkeley Campus

**Wednesday, August 15, 1984**

- 8:30-18:00 Second half of commercial exhibit—Room 120
- 8:30-10:10 *I. ATOMIC ADSORPTION*—L.M. Falicov, Presiding
- 8:30 I1 INV J.K. Nørskov and S. Holloway  
The Binding of Adsorbates to Metal Surfaces
- 9:10 I2 R.W. Godby, R. Haydock and V. Heine  
Bonding and Interaction of Oxygen Atoms on Nickel (001) from Self-Consistent Electronic Structure
- 9:30 I3 INV J.J. Barton, S.W. Robey, C.C. Bahr and D.A. Shirley  
Surface Structure Determination with ARPEFS
- 9:50 I4 INV E.L. Bullock, C.S. Fadley, B.L. Hermsmeier, M. Sagurton, R. Saiki, B. Sinkovic and R. Trehan  
Photoelectron Diffraction and Surface Structures: Future Prospects
- 10:10-10:40 COFFEE BREAK—Room 120
- 10:40-12:00 *J. SEMICONDUCTORS I*—X.D. Xie, Presiding
- 10:40 J1 INV Y.J. Chabal  
High-Resolution Infrared Spectroscopy and Surface Structure
- 11:20 J2 INV Y. Petroff  
Low-Temperature Photoemission on Semiconductors
- 11:40 J3 INV D. Vanderbilt and S.G. Louie  
Energy Minimization Calculations for Diamond (111) Surface Reconstructions
- 12:00-14:00 LUNCH BREAK
- 14:00-16:00 *K. ADSORBATE-ADSORBATE INTERACTIONS*—R.J. Madix, Presiding
- 14:00 K1 INV R.J. Birgeneau  
Phases and Phase Transitions in Systems with Competing Interactions
- 14:40 K2 J. Ochab, W.N. Unertl, P.H. Kleban, G. Akinci, P. Bak, N.C. Bartelt and T.L. Einstein  
The Ashkin-Teller Model and the Ordered Phases of Se/Ni(100)
- 15:00 K3 INV G. Ehrlich  
Surface Diffusion and Adatom-Adatom Interactions
- 15:40 K4 INV T.T. Tsong  
An Atom-Probe and Field Ion Microscope Study of the Atomic Structure and Composition of Metal Surfaces
- 16:00-16:30 INFORMAL RECEPTION—Room 120
- 16:00-18:00 *L. METALS AND ADSORBATES*—posters—Room 120
- L1 R. Richter, J.R. Smith and J.G. Gay  
Total Energies and Atom Locations at Solid Surfaces
- L2 K.M. Ho and K.P. Bohnen  
Investigations of Multilayer Relaxation on Metal Surfaces Using Self-Consistent Electronic Structure Calculations
- L3 H.L. Davis and G.-C. Wang  
Layer Relaxation of the Clean W(112) Surface and Its Variation with Adsorbed Oxygen
- L4 Y. Gauthier, Y. Joly, R. Baudoing and J. Rundgren  
Oscillatory Behavior of Some Surface Properties—Interlayer Distances in Metals and Composition in Binary Alloys
- L5 H.-J. Brocksch and K.H. Bennemann  
Theoretical Study of the Structural Stability of the Reconstructed (110)-Surfaces of Ir, Pt, and Au

- L6 T. Takai, T. Halicioglu and W.A. Tiller  
The Structure and Surface Energy of Au(110): Studied by Monte Carlo Method
- L7 C.-M. Chan and M.A. Van Hove  
A Comparison of the Missing-Row Model and Several Proposed Models  
for the Reconstructed Ir(110)-(1×2) Surface
- L8 U. Bardi, M. Torrini, E. Zanazzi, G. Rovida, M. Maglietta, P.N. Ross  
and M.A. Van Hove  
Structure of the Pt<sub>x</sub>Ti(001) Surface by LEED Dynamical Intensity Analysis
- L9 A.D. Tanner, K.T. Gillen, T.C.M. Horn, J. Los and A.W. Kleyn  
Surface Rainbow Scattering of Alkali Ions from W(110)
- L10 S.H. Overbury, D.R. Huntley and W.E. Brower, Jr.  
Structural Studies of the Surface of Amorphous Fe<sub>80</sub>B<sub>20</sub> by  
Low Energy Alkali Ion Scattering
- L11 S.H. Overbury, B.M. DeKoven and P.C. Stair  
Low Energy Alkali Ion Scattering as a Probe of Adsorbate Ordering
- L12 C. Umrigar and J.W. Wilkins  
Determination of the Geometry of Adsorbates on Surfaces Via Total  
Energy Calculations: H/Ni(100)
- L13 M.S. Daw and S.M. Foiles  
Application of the Embedded Atom Method to H on Ni and Pd Surfaces
- L14 M. Sagurton, E.L. Bullock and C.S. Fadley  
Single-Scattering Analysis of Off-Normal Photoelectron Diffraction Data
- L15 W.N. Mei, H.C. Poon and S.Y. Tong  
Fourier Transformation of Dynamical and Kinematical Energy Dependent  
Photoelectron Diffraction (EDPD) Spectra—A Theoretical Analysis
- L16 I.P. Batra, T. Engel and K.H. Rieder  
Helium Diffraction from Oxygen Covered Nickel Surfaces
- L17 P.S. Bagus, C.W. Bauschlicher, Jr. and C.J. Nelin  
Scattering of He from O/Ni(100): Cluster Model Studies
- L18 C.W. Bauschlicher, Jr., P.S. Bagus and K.E. Hermann  
The Bonding of Closed Shell Molecules to Transition Metal Surfaces
- L19 D. Tománek and K.H. Bennemann  
Total Energy Calculations for the Adsorption of N<sub>2</sub> and NO on Fe(111)
- L20 M.A. Passler  
Surface Structure of NO Adsorbed on Ni(011)
- L21 C.M. Mate and G.A. Somorjai  
Surface Structure of Fluorobenzene, Chlorobenzene, and Pyridine  
Adsorbed on Rh(111) Studied by HREELS
- L22 D.F. Ogletree, M.A. Van Hove and G.A. Somorjai  
Low-Energy Electron Diffraction Study of the Structure of Benzene  
Adsorbed on Pt(111)
- L23 J.L. Stickney, S.D. Rosasco, G.N. Salaita and A.T. Hubbard  
Ordered Ionic Layers Formed on Pt(111) from Aqueous Solutions
- L24 A.P. Alivisatos, D.H. Waldeck and C.B. Harris  
The Electronic Structure of Metals and Their Ability to Quench  
Molecular Excited States
- L25 G.M. Goncher, C.A. Parsons and C.B. Harris  
Surface Resonance Enhanced Multiphoton Fragmentation on Rough Metal Surfaces

**Thursday, August 16, 1984**

- 8:30-17:30 Continuation of second half of exhibit—Room 120
- 8:30-10:10 *M. SEMICONDUCTORS II*—D.R. Hamann, Presiding
- 8:30 M1 INV M.L. Cohen  
Theory of Surface Reconstruction
- 9:10 M2 INV E.G. McRae  
Triangle-Dimer Stacking-Fault Model of the Si(111)-(7×7) Surface Bonding Configuration
- 9:50 M3 INV P. Chiaradia  
Optical Transitions and Surface Structure
- 10:10-10:40 COFFEE BREAK—Room 120
- 10:40-12:00 *N. ORDERING*—J.B. Pendry, Presiding
- 10:40 N1 INV S.C. Fain, Jr. and H. You  
LEED Studies of Structures and Phase Transitions of Physically Adsorbed Nitrogen and Carbon Monoxide Molecules on Graphite
- 11:20 N2 INV M.B. Webb  
LEED Studies of Physisorbed Noble Gases on Metals and the Interadatom Interactions
- 11:40 N3 S. Brennan, P.H. Fuoss and P. Eisenberger  
X-Ray Scattering Studies of the Structure and Melting of Pb on Cu (110) Surfaces
- 14:00-15:40 *O. INTERFACES*—R.Z. Bachrach, Presiding
- 14:00 O1 INV L.M. Falicov and R. Victoria  
Magnetic Properties of Transition Metal Surfaces and Overlays
- 14:20 O2 INV P.H. Citrin  
Current Status and Future Directions of Surface-EXAFS
- 15:00 O3 INV F.A. Ponce  
Direct Observation of the Structure of Interfaces Using Atomic-Resolution Electron Microscopy
- 15:40-16:10 REFRESHMENTS—Room 120
- 16:10-17:30 *P. METAL RECONSTRUCTION*—D.J. Chadi, Presiding
- 16:10 P1 INV I.K. Robinson  
Surface Structure by X-Ray Diffraction
- 16:50 P2 INV R.F. Willis  
W(100) Surface Structural Phase Transformations: Current Models, Theory and Experiments
- 17:30 END OF ICSOS-1

JAN 22 1985

Abstract of Proceedings

These Proceedings are a collection of selected papers presented at the First International Conference on the Structure of Surfaces (ICSOS-1). They assess the status of surface structural determination and the relationship between surface or interface structures and physical or chemical properties of interest. This includes solid and adsorbate-covered surfaces, well-established and promising new surface-sensitive techniques, experiment and theory.

FIRST INTERNATIONAL CONFERENCE  
ON THE STRUCTURE OF SURFACES (ICSOS)

ROSTER

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Berkeley, California

|   |  |
|---|--|
| Carolyn R. Aita<br>University of Wisconsin<br>Lab for Surface Studies & Material<br>P. O. Box 784<br>Milwaukee, WI 53201<br><br>(414) 963-4733                            | Paul S. Bagus<br>IBM Research Laboratory<br>K33/281, 5600 Cottle Road<br>San Jose, CA 95193<br><br>(408) 256-7663                                |
| Douglas C. Allan<br>University of Pennsylvania<br>Department of Physics<br>Philadelphia, PA 19104<br><br>(215) 898-5987   | John J. Barton<br>Bldg. 70A, Rm. 1115<br>Lawrence Berkeley Laboratory<br>Berkeley, CA 94720<br><br>(415) 486-5666                                |
| Lynn R. Allen<br>University of Washington<br>BG-10, Department of Chemistry<br>Seattle, WA 98195<br><br>(206) 545-2594  | Igor Bartos<br>University of Waterloo<br>Department of Applied Mathematics<br>Waterloo, Ontario N2L 3G1<br>CANADA<br><br>(519) 885-1211 ext 3471 |
| N. M. Amer<br>Lawrence Berkeley Laboratory<br>Bldg. 70, Room 110A<br>Berkeley, CA 94720<br><br>(415) 486-5601   | Inder P. Batra<br>IBM Corporation K33/281<br>5600 Cottle Road<br>San Jose, CA 95193<br><br>(408) 256-7325  |
| Masakazu Aono<br>National Institute for Research<br>in Inorganic Materials<br>1-1 Namiki, Sakura-Mura<br>Niihara-Gun, Ibaraki, 305, JAPAN<br><br>(0290) 51 3351, ext. 251 | Bauschlicher<br>NASA AMES<br>STC-230-3<br>Moffett Field, CA<br><br>(415) 965-6231  |
| Walter E. Atkinson<br>Riverside Research Institute<br>1701 North Fort Myer Drive<br>Arlington, VA 22180<br><br>(703) 522-2310   | R. Juergen Behm<br>University of Munchen, F.R.G.<br>Sophiensn. 11<br>D-8000 Munchen 2<br>WEST GERMANY  |
| Robert Z. Bachrach<br>Xerox, P.A.R.C.<br>3333 Coyote Hill Road<br>Palo Alto, CA 94304<br><br>(415) 494-4157   | Peter A. Bennett<br>Arizona State University<br>Physics Department<br>Tempe, AZ 85287<br><br>(602) 965-5218                                      |

Brian E. Bent  
MMRD, Building 62  
Lawrence Berkeley Laboratory  
Berkeley, CA 94720

(415) 486-5600

Robert J. Birgeneau  
Mass. Institute of Technology  
Department of Physics  
Room 13-2114  
Cambridge, MA 02139

(617) 253-4937

Gregory S. Blackman  
MMRD, Building 62  
Lawrence Berkeley Laboratory  
Berkeley, CA 94720

(415) 486-5600

Richard J. Blake  
SERC Daresbury Laboratory  
Daresbury, Warrington  
Cheshire WA4 4AD  
ENGLAND

0925 65000

Charles Bonapace  
Princeton University  
Department of Electrical  
Engineering & Computer Science  
Princeton, NJ 08544

(609) 452-4642

Alexander M. Bradshaw  
Fritz-Haber Institute  
Faradayweg 4-6  
1000 Berlin 33  
WEST GERMANY

(30) 83 05 501

Ross D. Bringans  
Xerox P.A.R.C.  
3333 Coyote Hill Road  
Palo Alto, CA 94304

(415) 494-4156

Hans-Joachim R. Brocksch  
Freie Universitat Berlin  
FB20 WE 05  
Arnimallee 14  
D-1000 Berlin 33, W. GERMANY

Eric Bullock  
2545 The Mall  
University of Hawaii  
Honolulu, HI 96822

(808) 948-7380

Gianluigi Casalone  
University of Milano  
Dipartimento di Chimica Fisica  
Via Golgi 19  
Milano 20133, ITALY

(02) 292900

Yves J. Chabal  
AT&T Bell Laboratories  
600 Mountain Avenue, MH1C-333  
Murray Hill, NJ 07974

(201) 582-4193

D. J. Chadi  
Xerox, Palo Alto Research Center  
3333 Coyote Hill Road  
Palo Alto, CA 94304

(415) 969-4499

Chi Ming Chan  
Raychem Corporation  
300 Constitution Drive  
Menlo Park, CA 94025

(415) 361-5351

Cheng-Hsuan Chen  
AT&T Bell Laboratories  
600 Mountain Avenue  
Murray Hill, NJ 07974

(201) 582-7923

Shirley Chiang  
IBM Research Laboratory  
K33/281, 5600 Cottle Road  
San Jose, CA 95193

(408) 256-7318

Pietro Chiaradia  
CNR - Italy  
Via E. Fermi 38  
Frascati, Rome 00044

(06) 9426335

Paul H. Citrin  
AT&T Bell Laboratories  
100 Mountain Avenue  
Murray Hill, NJ 07974

(201) 582-5275

Marvin L. Cohen  
University of California-Berkeley  
Department of Physics  
Berkeley, CA 94720

(415) 642-4753

Philip I. Cohen  
University of Minnesota  
123 Church Street, SE  
Minneapolis, MN 55455

(612) 373-2577

Warren Eugene Collins  
Southern University  
Baton Rouge, LA 70813

(504) 771-4130

Edward H. Conrad  
University of Washington  
BG-10, Chemistry Department  
Seattle, WA 98185

(206) 545-2594

Matthew W. Copel  
Department of Physics  
University of Pennsylvania  
209 South 33rd Street  
Philadelphia, PA 19104

(215) 898-7943

Renee D. Diehl  
University of Liverpool  
Department of Physics  
Oliver Lodge Laboratory  
Liverpool L69 3BX, ENGLAND

(051) 709-6022, ext. 2247

Charles B. Duke  
Xerox Webster Research Center  
800 Phillips Road, 114  
Webster, NY 14580

(716) 422-2109

Juergen Eckert  
Los Alamos National Laboratory  
Mail Stop H 805, P-8  
Los Alamos, NM 87545

(505) 667-6069

William F. Egelhoff, Jr.  
Surface Science Division  
National Bureau of Standards  
Gaithersburg, MD 20899

(301) 921-2788

Adolfo G. Equiluz  
University of California-Irvine  
Department of Physics  
Irvine, CA 92717

(714) 856-6250

Gert Ehrlich  
Coordinated Science Laboratory  
University of Illinois  
1101 West Springfield Avenue  
Urbana, IL 61801

(217) 333-6448

M. El-Batanouny  
Boston University  
590 Commonwealth Avenue  
Boston, MA 02215

(617) 353-4721

Charles S. Fadlem  
Chemistry Department  
2545 The Mall  
University of Hawaii  
Honolulu, HI 96822

(808) 948-6401

Sam Fain  
Univesity of Washington  
Physics Department  
Seattle, WA 98195

(206) 543-5729

L. M. Falicov  
Department of Physics  
University of California  
Berkeley, CA 94720

(415) 642-5993

Helen H. Farrell  
Bell Communications Research  
600 Mountain Avenue  
Murray Hill, NJ 07928

(201) 582-3791

T. E. Felter  
Sandia  
Livermore, CA 94550

(415) 443-7399

Salvador Ferrer  
Univ. Auton. of Madrid  
Cantoblanco  
Madrid 34  
SPAIN

734-0100, ext. 1758

William Fink  
Department of Chemistry  
University of California-Davis  
Davis, CA 95616

(916) 753-5717

Michael Fluss  
Argonne National Laboratory  
9700 S. Cass Avenue  
Argonne, IL 60514

(312) 972-5149

Stephen M. Foiles  
Sandia Lational Laboratories  
Livermore, CA 94596

(415) 422-2898

Robert F. Frindt  
Physics Department  
Simon Fraser University  
Burnaby, BC V5A 156, CANADA

(604) 291-3161 or 291-3703

Paul H. Fuoss  
AT&T Bell Laboratories  
4B415, Crawfords Corner Road  
Holmdel, NJ 07733

(201) 949-3581

Eric Garfunkel  
Rutgers University  
New Brunswick, NJ 08903

(201) 932-2216

Stephen H. Garofalini  
Rutgers University  
Department of Ceramics  
P.O. Box 909  
Piscataway, NJ 08854

Edward L. Garwin  
 Stanford Linear Accelerator Center  
 P. O. Box 4349, Bin 72  
 Stanford, CA 94305

(415) 854-3300, ext. 2415

Burl M. Hall  
 Department of Physics  
 University of California-Irvine  
 Irvine, CA 92717

(714) 856-5453

Jack G. Gay  
 General Motors Research Labs.  
 Physics Department  
 Warren, MI 48090-9055

(313) 575-2898

Donald R. Hamann  
 AT&T Bell Laboratories  
 600 Mountain Avenue  
 Murray Hill, NJ 07974

(201) 582-4454

Walter M. Gibson  
 State University of N.Y.-Albany  
 Department of Physics  
 1400 Washington Avenue  
 Albany, NY 12722

(518) 457-8305

Dan Haneman  
 University of New South Wales  
 School of Physics  
 P. O. Box 1  
 Kensington, NSW 2033  
 AUSTRALIA

Rex W. Godby  
 Cavendish Laboratory  
 Madingley Road  
 Cambridge CB2 1RF  
 ENGLAND

(0223) 66477, ext. 415

Martin Henzler  
 Institut fur Festkorperphysik,  
 Universitat  
 Appelstr. 2  
 3000 Hannover, WEST GERMANY

49-511-762-4821

Torgny Gustafsson  
 University of Pennsylvania  
 Philadelphia, PA 19104

(215) 898-5953

Frank Herman  
 IBM Research Laboratory K32/281  
 5600 Cottle Road  
 San Jose, CA 95193

(408) 256-6254

Jochen Haase  
 Fritz-Haber Inst. der MPG  
 4-6 Faradayweg  
 1000 Berlin 33  
 WEST GERMANY

Kai-Ming Ho  
 Ames Laboratory, Physics Dept.  
 Iowa State University  
 Ames, IA 50011

(515) 294-1960; 294-7712

Timur Halicioglu  
 Stanford University (ELORET)  
 Stanford, CA 94305

(415) 497-3268

R. Howell  
 Lawrence Livermore National Lab.  
 Livermore, CA 94550

(415) 422-1977

Tung Hsu  
Arizona State University  
Department of Physics  
Tempe, AZ 85287

(602) 965-3561

Gen-you Hu  
Physics Department  
Brown University  
Providence, RI 02912

A. Norman Jette  
The Johns Hopkins Univ.  
Applied Physics Laboratory  
Johns Hopkins Road  
Laurel, MD 20707

(301) 953-6263

Harald Ibach  
IGV/KFA Julich  
Postfach 1913  
D-5170 Julich  
WEST GERMANY

2461/614561

Alex Ignatiev  
University of Houston  
Department of Physics  
University Park  
Houston, TX 77004

(713) 749-3889

Jisoon Ihm  
Bell Communications Research  
65 Tussel Lane  
Scotch Plains, NJ 07076

(201) 582-2884

Thomas E. Jackman  
Chalk River Nuclear Laboratories  
Solid State Science  
Chalk River, Ontario K0J 1J0  
CANADA

(613) 584-3311 ext. 2357

Les Jenkins  
Oak Ridge National Laboratory  
Building 3025, P. O. Box X  
Oak Ridge, TN 37831

John D. Joannopoulos  
Massachusetts Inst. of Technology  
77 Massachusetts Avenue, 12-116  
Cambridge, MA 02139

(617) 253-4806

Robert L. Johnson  
Max-Planck Institut  
Heisenbergstr. 1  
D-7000 Stuttgart 80  
WEST GERMANY

0711 6860 626

Franco P. Jona  
State University of New York  
Department of Materials Science  
Stony Brook, NY 11794

(516) 246-7649

Donald S. Kaufman  
University of Washington  
BG-10, Department of Chemistry  
Seattle, WA 98195

(206) 545-2954

Efthimios Kaxiras  
Massachusetts Inst. of Technology  
77 Massachusetts Avenue  
Room 12-128B  
Cambridge, MA 02139

(617) 253-5947

Robert E. Kirby  
Stanford Linear Accelerator Center  
Mail Stop 74  
P.O. Box 4349  
Stanford, CA 94305

(415) 854-3300, ext. 2795

Ondrej L. Krivanek  
Center for Solid State Science  
Arizona State University  
Tempe, AZ 85287

(602) 965-7512

Jean C. Lapujoulade  
CEN Saclay DPhG-PAS  
GIF sur Yvette Cedex 91191  
FRANCE

(6) 908-25-33

Le Lay  
CNRS - CRNCZ  
Campus de Luminy Case 913  
Marseille  
FRANCE

Keum H. Lee  
University of Missouri  
Department of Physics  
Columbia, MO 65211

(314) 882-6735 or 882-3434

Steven Levine  
Rutgers University  
Brett Road  
Biscataway, NJ 08854

(201) 932-2216

Joe C. H. Li  
Microlinear  
San Jose, CA

(408) 262-5200, ext. 535

Keng-San Liang  
Exxon Research & Engineering Co.  
Rt. 22 East, Clinton Township  
Annandale, NJ 08801

(201) 730-3032

Ingolf Lindau  
Stanford University  
Stanford Electronics Laboratories  
Stanford, CA 94305

(415) 497-1052

Frederick W. Lipps  
University of Houston, Energy Lab.  
4801 Calhoun St., Bldg. SPA  
Houston, TX 77004

(713) 749-1155

Gu Liu  
Lawrence Berkeley Laboratory  
1 Cyclotron Road, 70A-1115  
Berkeley, CA 94720

(415) 486-5666

Steven G. Louie  
University of California  
Department of Physics  
Berkeley, CA 94720

(415) 642-1709

Theodore E. Madey  
National Bureau of Standards  
Chemistry Building, Room B248  
Washington, DC 20234

(301) 921-2188

Robert J. Madix  
Stanford University  
Department of Chemical Engineering  
Stauffer III  
Stanford, CA 94305

(415) 497-2402 or 497-4906

Richard G. Masters  
Harris Semiconductor  
Analytical Services Dept.  
P.O. Box 883, M.S. 62-007  
Melbourne, FL 32901

(305) 724-7283

C. Mathew Mate  
MMRD, Building 62  
Lawrence Berkeley Laboratory  
Berkeley, CA 94720

(415) 486-5600

E. G. McRae  
AT&T Bell Laboratories  
Murray Hill, NJ 07974

(201) 582-4738

Michael J. Mehl  
Sachs Freeman Associates  
c/o Naval Research Laboratory  
Code 6684  
Washington, DC 20735

(202) 767-3934

Eugene C. Mele  
University of Pennsylvania  
Department of Physics  
Philadelphia, PA 19104

(215) 898-3135

P. Meyer  
Lawrence Livermore National Lab.  
P.O. Box 808  
Livermore, CA 94550

(415) 422-9678

Christian J. Minot  
Universite de Paris-Sud  
Orsay, 91405 FRANCE

33(6) 941-61-75

Winfried Monch  
University of Duisburg  
Bismarckstr. 81  
D-4100 Duisburg  
WEST GERMANY

(0203) 379-3265

Hans Morawitz  
IBM Research Lab, Department K33  
5600 Cottle Road  
San Jose, CA 95193

(408) 256-2174

Raymond Moreh  
Ben-Gurion University of Negev  
Physics Department  
Beer-Sheva 84120  
ISRAEL

Bernard J. Mrstik  
Naval Research Laboratory  
Code 6834  
Washington, DC 20375

(202) 767-3414

Klaus E. Muller  
University of Erlangen  
Erwin-Rommel-Str. 1  
Lehrstuhl fur  
Festkorperphysik  
Erwin-Rommel-Str. 1  
D8520 Erlangen, WEST GERMANY

Lee E. Myers  
USAF Office of Scientific Research  
AFOSR/NC  
Bolling AFB, DC 20332

(202) 767-4963

Seido Nagano  
Univ. of Wisconsin-Milwaukee  
Milwaukee, WI 53211

(414) 963-4969

Connie J. Nelin  
Analatom Inc  
253 Humboldt Court  
Sunnyvale, CA 94082

(415) 965-6231

Jacqueline M. Nicol  
University of Durham, UK  
c/o Los Alamos Nat'l Laboratory  
Mail Stop H805  
Los Alamos, NM 87545

(505) 667-6069

Osamu Nishikawa  
Tokyo Institute of Technology  
Dept. of Mat. Sci. & Eng.  
4259 Nagatsuta, Midori-ku  
Yokohama 227, JAPAN

(045) 922-1111 Ext. 2621

John Noonan  
Oak Ridge National Laboratory  
Building 3025 - P. O. Box X  
Oak Ridge, TN 37831

Peter J. A. Nordlander  
Chalmers University  
S-412 96 Gothenburg  
SWEDEN

David Norman  
Daresbury Laboratory  
S.E.R.C.  
Warrington WA4 4AD  
UNITED KINGDOM

(925) 65000

Jens K. Norskov  
NORDITA  
Blegdamsvej 17  
DK-2100 Copenhagen  
DENMARK

(1) 421616

John E. Northrup  
Xerox, Palo Alto Research Center  
3333 Coyote Hill Road  
Palo Alto, CA 94304

(415) 494-4187

David F. Ogletree  
MMRD, Building 62  
Lawrence Berkeley Laboratory  
Berkeley, CA 94720

(415) 486-6067

Marjorie A. Olmstead  
Larence Berkeley Laboratory  
Bldg. 70, Rm. 110  
Berkeley, CA 94720

(415) 486-5809

John Osen  
University of Washington  
Physics Department  
Seattle, WA 98195

(206) 543-5729

Steven H. Overbury  
Oak Ridge National Laboratory  
P. O. Box X  
Oak Ridge, TN 37831

(615) 574-5040

Juan Parellada-Sabata  
Facultat de Fisica  
Universitat de Barcelona  
Diagonal 645  
Barcelona 28, SPAIN

(343) 330.73.11 ext 242

Bradford B. Pate  
SSRL, Stanford University  
SLAC Bin 69, PO Box 4349  
Stanford, CA 94305

(415) 854-3300 x3445

John B. Pendry  
Imperial College  
Department of Physics  
Prince Consort Road  
London SW7 2BZ, ENGLAND

(01) 589-5111, ext 2304

Piero Pianetta  
Stanford University  
SLAC - Bin 69  
P.O. Box 4349  
Stanford, CA 94305

(415) 854-3300, ext. 3484

Joseph Pimbley  
General Electric/RPI  
15 Cheshire Place  
Schenectady, NY 12309

(518) 393-0890

Fernando A. Ponce  
Xerox Palo Alto Research Center  
3333 Coyote Hill Road  
Palo Alto, CA 94304

(415) 494-4199

Hin Chuck Poon  
Univ. of Wisconsin-Milwaukee  
Milwaukee, WI 53201

(414) 963-6082

Paul Pukite  
University of Minnesota  
123 Church Street, SE  
Minneapolis, MN

(612) 373-2482

Neville Vincent Richardson  
University of Liverpool  
Donnan Labs., Grove Street  
Liverpool L69 3BX  
UNITED KINGDOM

051-709-6022, ext. 2560

Steven L. Richardson  
Department of Physics  
Univ. of California at Berkeley  
Berkeley, CA 94720

(415) 642-1031, or 642-4753

Roy Richter  
General Motors Research Labs.  
Physics Department  
Warren, MI 48090-9055

(313) 575-2901

Ian K. Robinson  
Bell Laboratories  
Murray Hill, NJ 07974

(201) 582-6056

Lyle D. Roelofs  
University of Maryland  
Department of Physics & Astronomy  
College Park, MD 20742

(301) 454-7043

Ira J. Rosenberg  
Lawrence Livermore National Lab.  
Livermore, CA 94550

(415) 422-0684

Gerd M. Rosenblatt  
Chemistry Division  
Los Alamos National Laboratory  
CHM-DO, MS J563  
Los Alamos, NM 87545

(505) 667-6250

Gianfranco Rovida  
Dipartimento di Chimica  
Via G.Capponi 9  
50121 Firenze  
ITALY

240865

Jack E. Rowe  
Physics Department  
University of Florida  
Gainesville, FL 32611

(904) 392-0521 - (904) 392-7334

Jack E. Rowe  
University of Florida  
Department of Physics  
Gainesville, FL 32611  
  
(904) 392-7334 or 0521

Claude A. Sebenne  
Lab Physique des Solides  
Universite P. et M. Curie  
4 Place Jussieu  
75230 Paris CEDEX 05  
FRANCE

Takasi Sagawa  
Tohoku University  
Department of Physics  
Sendai 980  
JAPAN  
  
0222-22-1800, ext. 3239

Annabella Selloni  
Department of Physics  
University of Rome  
P22a A. Moro, 2  
00185 Roma  
ITALY

Dilano K. Saldin  
Imperial College of Science  
and Technology  
Prince Consort Road  
London SW7 2BZ, ENGLAND  
  
(01) 589-5111

Massimo Simonetta  
University of Milan  
Via Golgi 19  
20122 Milano  
ITALY

Lionel Salem  
Centre d'Orsay  
Universite de Paris-Sud  
Lab. de Chimie Theorique  
91405 Orsay  
FRANCE

Charles P. Slichter  
University of Illinois at Urbana  
1110 W. Green Street  
Urbana, IL 61801  
  
(217) 333-3834

David A. Saloner  
University of Wisconsin-Madison  
Materials Science Program  
1111 ERB, 1500 Johnson Drive  
Madison, WI 53706  
  
(608) 263-2089

Leon Smit  
FOM Institute for Atomic and  
Molecular Physics  
P.O. Box 41883  
1009 DB Amsterdam  
THE NETHERLANDS

Robert Schlogl  
University of Basle  
Ulingelsergstr. 82  
CH 4056 Basle  
SWITZERLAND

John R. Smith  
General Motors Research  
Physics Department  
Warren, MI 98090-9055

Matthias Schoebinger  
IBM San Jose/ K33-281  
5600 Cottle Road  
San Jose, CA 95193

Gabor A. Somorjai  
University of California  
Department of Chemistry  
Berkeley, CA 94720

(408) 256-2190

(415) 642-4053

William E. Spicer  
 Stanford University  
 Stanford Electronics Laboratories  
 McCullough Building #228  
 Stanford, CA 94305

(415) 497-4643

John L. Stickney  
 University of California  
 at Santa Barbara  
 Santa Barbara, CA 93106

(805) 961-3905

Joachim Stohr  
 Exxon Research & Engineering Co.  
 Annandale, NJ 08801

(516) 282-2070

Masaetsu Takahashi  
 #863 I House,  
 2299 Piedmont Avenue  
 Berkeley, CA 94720

(415) 643-3052

Takashi Takahashi  
 Tohoku University  
 Department of Physics  
 Sendai 980  
 JAPAN

0222-22-1800, ext. 3239

Tadayoshi Takai  
 Material Science and Engineering  
 Stanford University  
 Stanford, CA 94305

(415) 497-9497

Ariadne Tenner  
 FOM-Institute for Atomic and  
 Molecular Physics  
 Kruislaan 407  
 1098 SJ Amsterdam  
 THE NETHERLANDS

Jerry D. Tersoff  
 AT&T Bell Laboratories  
 600 Mountain Avenue, Room 7C325  
 Murray Hill, NJ 07974

(201) 582-7350

Patricia A. Thiel  
 Iowa State University  
 Ames, IA 50011

(515) 294-8985

Hiroshi Tochihara  
 The University of Tokyo  
 Institute for Solid State Physics  
 Roppongi 7-22-1, Minato-ku  
 Tokyo 106, JAPAN

3-476-6811 ext. 5302

David Tomanek  
 Freie Universitat Berlin, FB Physik  
 Arnimallee 14  
 Berlin 33 D-1000  
 WEST GERMANY

(030) 838-3797

David S. Y. Tong  
 Univ. of Wisconsin - Milwaukee  
 P.O. Box 413  
 Milwaukee, WI 53201

(414) 351-1389 or 963-4474

Ruud M. Tromp  
 IBM  
 Thomas J. Watson Research Center  
 P. O. Box 218  
 Yorktown Heights, NY 10598

(914) 945-1242

Tien T. Tsong  
 Pennsylvania State University  
 104 Davey Laboratory  
 University Park, PA 16802

(814) 865-2813

Roger Uhrberg  
Xerox, Palo Alto  
3333 Coyote Hill Road  
Palo Alto, CA 94304

(415) 494-4181

Cyrus J. Umrigar  
Cornell University  
Clark Hall - LASSP  
Ithaca, NY 14850

(607) 256-6487

William N. Unertl  
LASST, 2 Barrows Hall  
University of Maine  
Orono, ME 04469

(207) 581-2251

Thomas Upton  
Exxon Research & Engineering  
Rt. 22 East  
Annandale, NJ 08801

(201) 730-2555

Jan H. van der Merwe  
University of Pretoria  
Pretoria 0002, Transvaal  
SOUTH AFRICA

(012) 420 2459

Michel A. Van Hove  
MMRD, Building 62  
Lawrence Berkeley Laboratory  
Berkeley, CA 94720

(415) 486-6160

David Vanderbilt  
University of California  
Department of Physics  
Berkeley, CA 94720

(415) 642-1031

Randall H. Victora  
Department of Physics  
University of California  
Berkeley, CA 94720

(415) 642-5993

Arthur J. Viescas  
Stanford University  
251 McCullough - SEL  
Stanford, CA 94086

(415) 497-3209

Dennis T. Vigren  
University of the Saar  
Inst. fur Theor. Physik  
6600 Saarbrucken  
WEST GERMANY

(681) 302-3967

Ching-Ping S. Wang  
Department of Physics  
University of Maryland  
College Park, MD 20742

(301) 454-6628

Po-Kang Wang  
University of Illinois-Urbana  
Department of Physics  
1110 W. Green Street  
Urbana, IL 61801

(217) 333-4628

Sheng-Wei Wang  
Lawrence Berkeley Laboratory  
1 Cyclotron Road  
Berkeley, CA 94720

(415) 486-4821

Xun Wang  
Physics Department  
Fudan University  
Shanghai  
PEOPLE'S REPUBLIC OF CHINA

480906, ext. 172

Maurice B. Webb  
University of Wisconsin-Madison  
Physics Department  
Madison, WI 53705

(608) 233-6797

Jerry L. Whitten  
S.U.N.Y. at Stony Brook  
Chemistry Department  
Stony Brook, NY 11794

(516) 246-6068

R. Stanley Williams  
Univ. of Calif. at Los Angeles  
Department of Chemistry  
Los Angeles, CA 90024

(213) 825-8818

Roy F. Willis  
Cavendish Laboratory  
Department of Physics  
Madingley Road  
Cambridge CB3 OHE  
ENGLAND

R. J. Wilson  
IBM Research  
5600 Cottle Road  
San Jose, CA 95193

(408) 256-2491

Christopher J. Wright  
A.E.R.E. Harwell  
Building 521  
Didcot, Oxon. OX110RA  
ENGLAND

(0235) 21054, ext. 5208

Naijuan Wu  
University of Houston  
Department of Physics  
Houston, TX

Xide Xie  
Physics Department  
Fudan University  
Shanghai  
PEOPLE'S REPUBLIC OF CHINA

480906, ext. 172, 483331

Mu-Liang Xu  
Univ. of Wisconsin - Milwaukee  
Milwaukee, WI 53201

(414) 963-6082

Chia H. Yang  
Southern University  
Baton Rouge, LA 70813

(504) 771-4130

W. S. Yang  
Peking University  
Beijing  
CHINA

Jory Yarnoff  
UCLA, Chemistry Department  
405 Hilgard Avenue  
Los Angeles, CA 90024

(213) 206-8393

See-Chen Ying  
Brown University  
Providence, RI 02912

(401) 863-2684

Hoydoo You  
University of Washington  
Physics Department  
Seattle, WA 98195

(206) 543-5729

Aug 13 16:41 1984

ICSOS Roster

Page 15

Shengbai Zhang  
University of California-Berkeley  
Department of Physics  
Berkeley, CA 94720

(415) 642-2635

Paul R. Zschack  
Northwestern University  
2145 Sheridan Road  
Evanston, IL 60201

(312) 492-7677